

## ProtoTOX

ProtoTOX is a computational (*in silico*) tool focused on the prediction of endpoints related with the toxicity of chemical substances. It includes a variety of *in vitro* and *in vivo* tests in humans, animals, microorganisms and cell lines.

ProtoTOX mainly includes, but is not limited to, endpoints used by REACH, a European Union regulation, adopted to improve the protection of human health and the environment from the risks that can be posed by chemicals, while enhancing the competitiveness of the EU chemicals industry.

## Endpoint

### Human health effects: in vivo pre-natal-developmental

A reproductive and/or developmental toxic substance may affect fertility and can cause health effects in offspring after recurring contact by ingestion, inhalation, or skin contact. This study is designed to provide information on substance-induced effects on growth and survival of the foetuses, and increased incidences in external, skeletal and soft tissue malformations and variations in foetuses.

## Metrics

### Training set

| Experimental values | QSAR predictions |       |
|---------------------|------------------|-------|
|                     | non-toxic        | toxic |
| non-toxic           | 85               | 9     |
| toxic               | 28               | 107   |

### Validation set


| Experimental values | QSAR predictions |       |
|---------------------|------------------|-------|
|                     | non-toxic        | toxic |
| non-toxic           | 25               | 16    |
| toxic               | 26               | 34    |

| Parameters                       | Training | Validation |
|----------------------------------|----------|------------|
| Accuracy                         | 0.84     | 0.58       |
| Sensitivity / recall             | 0.79     | 0.57       |
| Specificity                      | 0.90     | 0.61       |
| Precision                        | 0.92     | 0.68       |
| Negative predictive value        | 0.75     | 0.49       |
| F-score                          | 0.85     | 0.62       |
| Matthews Correlation Coefficient | 0.69     | 0.17       |
| Critical Success Index           | 0.74     | 0.45       |
| Area under the ROC               | 0.85     | 0.59       |

ProtoTOX is part of



ProtoPRED platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, by proprietary (Q)SAR models.

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